

Surface Structure via Photoelectron Diffraction of Surface Core Level States

M.Stichler¹, W. Wurth¹, D. Menzel¹, R. Denecke^{2,3} and C.S. Fadley^{2,3}

¹Physik-Department E20, Technische Universität München,
Garching 85747, Germany

²Materials Science Division, Ernest Orlando Lawrence Berkeley National Laboratory,
University of California, Berkeley, California 94720, USA

³Department of Physics, University of California at Davis,
Davis CA 95616, USA

INTRODUCTION

At the ALS bending magnet beamline 9.3.2 and using its Advanced Photoelectron Spectrometer/Diffractometer experimental endstation [1], we have measured high-resolution photoemission spectra of the Ru-3d_{5/2} core level for the clean Ru(001) surface, as well as covered by several adsorbates. The surface core level shift (SCLS) of the clean surface and the adsorbate-induced SCLS's due to H, O, CO, NO, and coadsorption layers were distinct, and the latter proved to be adsorbate-specific. In the next step, we measured the same spectra as functions of the electron emission angle and of the photon energy for the clean and the O covered Ru(001) surface with the aim of attaining a structure determination via photoelectron diffraction.

SURFACE CORE LEVEL STATES

Fig.1 depicts high resolution ($E/\Delta E > 5000$)

3d_{5/2} core level spectra for the clean and adsorbate-covered surfaces. It is evident that each spectrum is composed of at least two components. Focusing on the core level spectra of the clean surface (see the spectrum at the bottom) the deconvolution indicates three states - B, S1 and S2 - separated in binding energy by 363 and 135 meV, respectively. For the identification of the surface and bulk states the simplest way is the comparison with the adsorbate covered surfaces. B is the only state whose binding energy does not change upon adsorption and thus can be assigned to the bulk state. S1 and S2, whose binding energies vary with the different adsorbates must belong to layers close to the surface. Without restriction of generality it can be assumed that the distortion of the topmost surface layer is more pronounced than in sublayers. Consequently S1 can be related to the top layer and S2 to a transition state between the surface and the bulk, most likely the second layer. In agreement with a model of Spanjaard et al. [2] S1 shifts energetically to lower binding energies for transition metals with more than half filled valence bands because of conservation of quasi-neutrality.

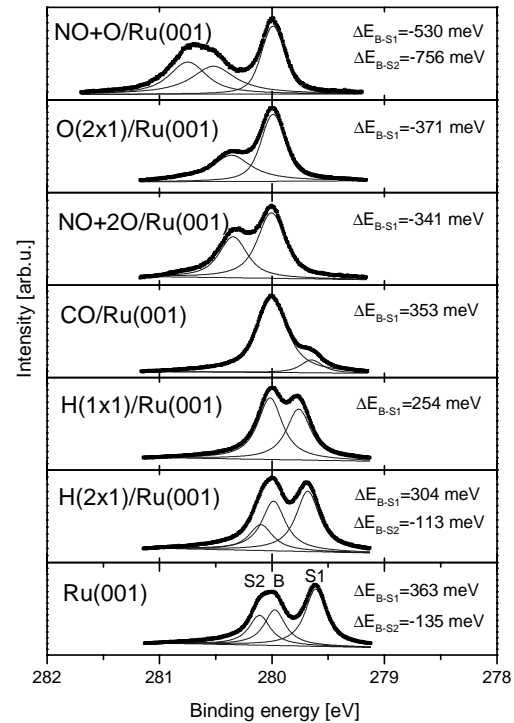


Figure 1: Surface core level shift: high resolution Ru-3d_{5/2}-XPS spectra measured at grazing incidence for the clean and several adsorbate covered (ordered overlayers) Ru(001) surfaces.

In the case of the adsorbate covered surfaces, which are all characterized by ordered superstructures, the most striking feature is the change in the position of the surface state with respect to the bulk state. The first class of adsorbates, which includes H and CO, shows an intermediate surface state between S1 and B of the clean surface, while the second class, comprising O and NO, induces a shift to higher binding energies of the surface state with respect to the bulk state. It is obvious that the surface core level spectra are sensitive and adsorbate specific for different adsorbate covered surfaces.

SURFACE STRUCTURE VIA PHOTOELECTRON DIFFRACTION

In the next step we measured angle and energy dependent photoelectron diffraction patterns for the clean and oxygen covered surfaces, aiming at direct structural determinations via the surface state S1 as well as via the bulk state B. For the O-covered layer we also measured the diffraction patterns of the O1s level for comparison with the Ru-3d_{5/2} results. In the case of the angle dependent measurements, the angle between the linearly polarized incident radiation and the electron emission direction was fixed at 70 degrees, with the sample being rotated around two perpendicular axes to obtain the full diffraction pattern. The photon energies used were 400 and 700 eV for the Ru-3d_{5/2} core level and 650 eV for O1s. In the case of the energy dependent measurements, we varied the excitation energy from 300 to 800 eV. We are presently working at the extraction of structural parameters from these diffraction patterns by comparing the experimental with theoretical results of multiple scattering calculations for scattered photoelectrons, via an R-factor analysis. The final results will be compared with LEED-IV results for the clean and the p(2x1)-O covered Ru(001) surfaces [3,4].

REFERENCES

1. Z. Hussain et al., J. Elec. Spec. and Rel. Phen. 80, 401 (1996)
C.S. Fadley et al., J. Elec. Spec. and Rel. Phen. 75, 273 (1995)
2. D. Spanjaard et al., Surf. Sci. Rep. 5, 1 (1985)
3. H. Pfnür et al., Surf. Sci. 220, 43 (1989)
4. M. Lindroos et al., Surf. Sci. 222, 451 (1989)

This work has been supported by the Deutsche Forschungsgemeinschaft through project Me 266/22-1 and by DOE, OER, BES, Mat. Sci. Div. (Contract DE-AC03-76SF00098), ONR (Contract N00014-94-1-0162). R.D gratefully acknowledges a postdoctoral fellowship granted by the Deutsche Forschungsgemeinschaft.

Principal investigator: Dietrich Menzel, Physik-Department E20, Technische Universität München, Garching 85747, Germany. E-mail: menzel@e20.physik.tu-muenchen.de.